Connecting via Winsock to STN

Welcome to STN International! Enter x:X

LOGINID:SSPTASMR1614

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	DEC 01	ChemPort single article sales feature unavailable
NEWS	3	APR 03	CAS coverage of exemplified prophetic substances enhanced
NEWS	4	APR 07	STN is raising the limits on saved answers
NEWS	5	APR 24	CA/CAplus now has more comprehensive patent assignee information
NEWS	6	APR 26	USPATFULL and USPAT2 enhanced with patent assignment/reassignment information
NEWS	7	APR 28	CAS patent authority coverage expanded
NEWS	8	APR 28	ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS	9	APR 28	Limits doubled for structure searching in CAS REGISTRY
NEWS	10	MAY 08	STN Express, Version 8.4, now available
NEWS	11	MAY 11	STN on the Web enhanced
NEWS	12	MAY 11	BEILSTEIN substance information now available on STN Easy
NEWS	13	MAY 14	DGENE, PCTGEN and USGENE enhanced with increased limits for exact sequence match searches and introduction of free HIT display format
NEWS	14	MAY 15	INPADOCDB and INPAFAMDB enhanced with Chinese legal status data
NEWS	15	MAY 28	CAS databases on STN enhanced with NANO super role in records back to 1992
NEWS	16	JUN 01	CAS REGISTRY Source of Registration (SR) searching enhanced on STN

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN customer agreement. This agreement limits use to scientific research. Use for software development or design, implementation of commercial gateways, or use of CAS and STN data in the building of commercial products is prohibited and may result in loss of user privileges and other penalties.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

```
FILE 'HOME' ENTERED AT 12:00:09 ON 02 JUN 2009

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.88       0.88

FILE 'REGISTRY' ENTERED AT 12:02:15 ON 02 JUN 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2009 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:    1 JUN 2009  HIGHEST RN 1151607-22-5
DICTIONARY FILE UPDATES:   1 JUN 2009  HIGHEST RN 1151607-22-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\STNEXP\Queries\10564010 str 1.str

L1      STRUCTURE UPLOADED

=> s l1 sss full
FULL SEARCH INITIATED 12:02:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       88 TO ITERATE

100.0% PROCESSED       88 ITERATIONS                                0 ANSWERS
SEARCH TIME: 00.00.01

L2            0 SEA SSS FUL L1

=>
Uploading C:\Program Files\STNEXP\Queries\10564010 str 2.str

L3      STRUCTURE UPLOADED

=> s l3 sss full
FULL SEARCH INITIATED 12:13:31 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      633 TO ITERATE

100.0% PROCESSED      633 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

L4            3 SEA SSS FUL L3

=> d his
```

```
     (FILE 'HOME' ENTERED AT 12:00:09 ON 02 JUN 2009)

     FILE 'REGISTRY' ENTERED AT 12:02:15 ON 02 JUN 2009
L1              STRUCTURE UPLOADED
L2            0 S L1 SSS FULL
L3              STRUCTURE UPLOADED
L4            3 S L3 SSS FULL

=>  s l1 sss full
FULL SEARCH INITIATED 12:13:54 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -       88 TO ITERATE

100.0% PROCESSED       88 ITERATIONS                                 0 ANSWERS
SEARCH TIME: 00.00.01

L5            0 SEA SSS FUL L1

=> d l4 1-3 ibib ab hitstr
'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'AB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats.  The predefined substance formats
are:  (RN = CAS Registry Number)

REG    - RN
SAM    - Index Name, MF, and structure - no RN
FIDE   - All substance data, except sequence data
IDE    - FIDE, but only 50 names
SQIDE  - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD    - Protein sequence data, includes RN
SQD3   - Same as SQD, but 3-letter amino acid codes are used
SQN    - Protein sequence name information, includes RN

EPROP  - Table of experimental properties
PPROP  - Table of predicted properties
PROP   - EPROP, ETAG, PPROP and SPEC

Any CA File format may be combined with any substance format to
obtain CA references citing the substance.  The substance formats
must be cited first.  The CA File predefined formats are:

ABS  -- Abstract
APPS -- Application and Priority Information
BIB  -- CA Accession Number, plus Bibliographic Data
CAN  -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND  -- Index Data
IPC  -- International Patent Classification
PATS -- PI, SO
STD  -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented
```

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when
it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented,
with text labels.

For additional information, please consult the following help
messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):d 14 1-3 ibib ab hitstr
'D' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats. The predefined substance formats
are: (RN = CAS Registry Number)

REG   - RN
SAM   - Index Name, MF, and structure - no RN
FIDE   - All substance data, except sequence data
IDE   - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD   - Protein sequence data, includes RN
SQD3   - Same as SQD, but 3-letter amino acid codes are used
SQN   - Protein sequence name information, includes RN

EPROP - Table of experimental properties
PPROP - Table of predicted properties
PROP   - EPROP, ETAG, PPROP and SPEC

Any CA File format may be combined with any substance format to
obtain CA references citing the substance. The substance formats
must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when
it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented,
with text labels.

For additional information, please consult the following help
messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):file caplus
'FILE' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'CAPLUS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'

The following are valid formats:

Substance information can be displayed by requesting individual
fields or predefined formats. The predefined substance formats
are: (RN = CAS Registry Number)

REG   - RN
SAM   - Index Name, MF, and structure - no RN
FIDE   - All substance data, except sequence data
IDE   - FIDE, but only 50 names
SQIDE - IDE, plus sequence data
SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used
SQD   - Protein sequence data, includes RN
SQD3   - Same as SQD, but 3-letter amino acid codes are used
SQN   - Protein sequence name information, includes RN

EPROP - Table of experimental properties
PPROP - Table of predicted properties
PROP   - EPROP, ETAG, PPROP and SPEC

Any CA File format may be combined with any substance format to
obtain CA references citing the substance. The substance formats
must be cited first. The CA File predefined formats are:

ABS -- Abstract
APPS -- Application and Priority Information
BIB -- CA Accession Number, plus Bibliographic Data
CAN -- CA Accession Number
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)
IND -- Index Data
IPC -- International Patent Classification
PATS -- PI, SO
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels
IBIB -- BIB, indented, with text labels
ISTD -- STD format, indented

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when
it is available.
The MAX format is the same as ALL.
The IALL format is the same as ALL with BIB ABS and IND indented,
with text labels.

For additional information, please consult the following help
messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):end

=> file caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                         ENTRY   SESSION
FULL ESTIMATED COST   567.24   568.12

FILE 'CAPLUS' ENTERED AT 12:15:51 ON 02 JUN 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 2 Jun 2009 VOL 150 ISS 23
FILE LAST UPDATED: 1 Jun 2009 (20090601/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l4
L6   1 L4

=> s l6 ibib ab hitstr
MISSING OPERATOR L6 IBIB
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> d l6 ibib ab hitstr

L6   ANSWER 1 OF 1 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:120898 CAPLUS
DOCUMENT NUMBER: 142:219297
TITLE: Preparation of pyrimidine analogs as 5-HT2b receptor antagonists
INVENTOR(S): Borman, Richard Anthony; Coleman, Robert Alexander; Clark, Kenneth Lyle; Oxford, Alexander William; Hynd, George; Archer, Janet Ann; Aley, Amanda; Harris, Neil Victor
PATENT ASSIGNEE(S): Pharmagene Laboratories Limited, UK
SOURCE: PCT Int. Appl., 173 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

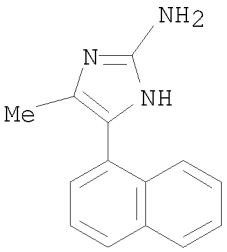
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2005012263	A1	20050210	WO 2004-GB3184		20040723
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2532505	A1	20050210	CA 2004-2532505		20040723
EP 1648876	A1	20060426	EP 2004-743517		20040723
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK					
JP 2006528617	T	20061221	JP 2006-520897		20040723
US 20090018150	A1	20090115	US 2006-564010		20060111
PRIORITY APPLN. INFO.:			GB 2003-17346	A	20030724
			US 2003-490286P	P	20030728
			WO 2004-GB3184	W	20040723

OTHER SOURCE(S): CASREACT 142:219297; MARPAT 142:219297

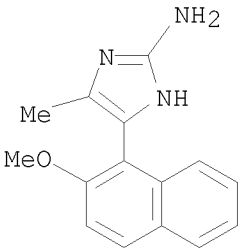
AB Title compds. represented by the formula I [wherein X = O or NH; R1 = (un)substituted aryl; R2, R3 = independently H, (un)substituted (cyclo)alkyl, cycloalkylalkyl, phenylalkyl; R4, R5 = independently H, (un)substituted (phenyl)alkyl, sulfonylalkyl, carbonylalkyl, alkylamino or R4R5 = (un)substituted heterocyclic group; and pharmaceutically acceptable salts or solvates thereof], and 3 addnl. Markush structures, were prepared as 5-HT2b receptor agonists. For example, reaction of 2-amino-4-chloro-6-methylpyrimidine with aniline in the microwave cavity gave II. I were tested for binding activity of 5-HT2A, 5-HT2B and 5-HT2C. Thus, I and their pharmaceutical compns. are useful for the treatment of a condition alleviated by antagonism of a 5-HT2B receptor, such as digestive tract disease (no data).

IT 842155-08-2P 842155-11-7P 842155-12-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinyl, imidazolyl, oxazolyl and triazolyl amine derivs. as 5-HT2b receptor antagonists)

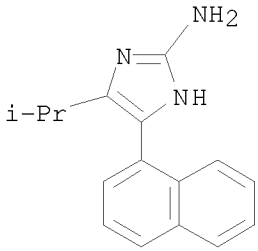
RN 842155-08-2 CAPLUS
CN 1H-Imidazol-2-amine, 4-methyl-5-(1-naphthalenyl)- (CA INDEX NAME)



RN 842155-11-7 CAPLUS
CN 1H-Imidazol-2-amine, 5-(2-methoxy-1-naphthalenyl)-4-methyl- (CA INDEX NAME)



RN 842155-12-8 CAPLUS
CN 1H-Imidazol-2-amine, 4-(1-methylethyl)-5-(1-naphthalenyl)- (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	17.64	585.76

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.82	-0.82

FILE 'REGISTRY' ENTERED AT 12:30:22 ON 02 JUN 2009

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 1 JUN 2009 HIGHEST RN 1151607-22-5
DICTIONARY FILE UPDATES: 1 JUN 2009 HIGHEST RN 1151607-22-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\STNEXP\Queries\10564010 str 3.str

L7   STRUCTURE UPLOADED

=> s l7 sss full
FULL SEARCH INITIATED 12:30:41 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   138545 TO ITERATE

100.0% PROCESSED   138545 ITERATIONS   58 ANSWERS
SEARCH TIME: 00.00.09

L8   58 SEA SSS FUL L7

=> file caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                   ENTRY   SESSION
FULL ESTIMATED COST   185.88   771.64

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)   SINCE FILE   TOTAL
                                                   ENTRY   SESSION
CA SUBSCRIBER PRICE   0.00   -0.82

FILE 'CAPLUS' ENTERED AT 12:31:04 ON 02 JUN 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 2 Jun 2009 VOL 150 ISS 23

FILE LAST UPDATED: 1 Jun 2009 (20090601/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=>
Uploading C:\Program Files\STNEXP\Queries\10564010 str 3.str

L9   STRUCTURE UPLOADED

=> file caplus
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                         ENTRY   SESSION
FULL ESTIMATED COST   1.50   773.14

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)   SINCE FILE   TOTAL
                                                         ENTRY   SESSION
CA SUBSCRIBER PRICE   0.00   -0.82

FILE 'CAPLUS' ENTERED AT 12:32:57 ON 02 JUN 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 2 Jun 2009 VOL 150 ISS 23
FILE LAST UPDATED: 1 Jun 2009 (20090601/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Feb 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Feb 2009

CAplus now includes complete International Patent Classification (IPC)
reclassification data for the third quarter of 2008.

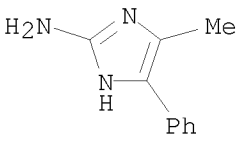
CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d his

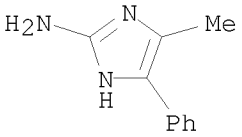
```
     (FILE 'HOME' ENTERED AT 12:00:09 ON 02 JUN 2009)

     FILE 'REGISTRY' ENTERED AT 12:02:15 ON 02 JUN 2009
L1             STRUCTURE UPLOADED
L2           0 S L1 SSS FULL
L3             STRUCTURE UPLOADED
L4           3 S L3 SSS FULL
L5           0 S L1 SSS FULL

     FILE 'CAPLUS' ENTERED AT 12:15:51 ON 02 JUN 2009
L6           1 S L4

     FILE 'REGISTRY' ENTERED AT 12:30:22 ON 02 JUN 2009
L7             STRUCTURE UPLOADED
L8          58 S L7 SSS FULL

     FILE 'CAPLUS' ENTERED AT 12:31:04 ON 02 JUN 2009
L9             STRUCTURE UPLOADED

     FILE 'CAPLUS' ENTERED AT 12:32:57 ON 02 JUN 2009

=> s l8
L10         17 L8

=> d l10 1-17 ibib ab hitstr

L10  ANSWER 1 OF 17  CAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:        2007:1474785  CAPLUS
DOCUMENT NUMBER:         148:239095
TITLE:                   An Efficient and Expeditious Synthesis of Di- and
                         Monosubstituted 2-Aminoimidazoles
AUTHOR(S):               Soh, Chai Hoon; Chui, Wai Keung; Lam, Yulin
CORPORATE SOURCE:        Dep. Chem., Natl. Univ. Singapore, 117543, Singapore
SOURCE:                  Journal of Combinatorial Chemistry (2008), 10(1),
                         118-122
                         CODEN: JCCHFF; ISSN: 1520-4766
PUBLISHER:               American Chemical Society
DOCUMENT TYPE:           Journal
LANGUAGE:                English
OTHER SOURCE(S):         CASREACT 148:239095
AB   A microwave-assisted protocol was developed for the construction of di-
     and monosubstituted 2-aminoimidazoles.  The two-step reaction involves the
     synthesis of N-(1H-imidazol-2-yl)acetamides from readily available
     α-haloketones and N-acetylguanidine, followed by deacetylation.
     Significant rate enhancement was observed for both steps of the protocol, and
     the overall reaction time was shortened to 20 min compared to 48 h of the
     conventional procedures.  A representative set of di- and monosubstituted
     2-aminoimidazoles was prepared using com. available parallel reactors.
IT   1006371-60-3P
     RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
        (preparation of di- and monosubstituted 2-aminoimidazoles by
        microwave-assisted preparation of N-(1H-imidazol-2-yl)acetamides from
        α-haloketones and N-acetylguanidine followed by deacetylation)
RN   1006371-60-3  CAPLUS
CN   1H-Imidazol-2-amine, 4-methyl-5-phenyl-, hydrochloride, hydrate (1:1:2)
     (CA INDEX NAME)
```



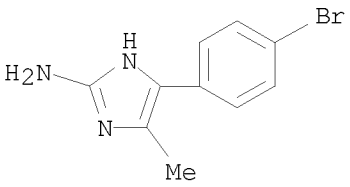
● HCl

● 2 H_2O

IT 6646-81-7P 1006371-59-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of di- and monosubstituted 2-aminoimidazoles by microwave-assisted preparation of N-(1H-imidazol-2-yl)acetamides from α-haloketones and N-acetylguanidine followed by deacetylation)
RN 6646-81-7 CAPLUS
CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl- (CA INDEX NAME)



RN 1006371-59-0 CAPLUS
CN 1H-Imidazol-2-amine, 5-(4-bromophenyl)-4-methyl- (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:120898 CAPLUS
DOCUMENT NUMBER: 142:219297
TITLE: Preparation of pyrimidine analogs as 5-HT2b receptor antagonists
INVENTOR(S): Borman, Richard Anthony; Coleman, Robert Alexander; Clark, Kenneth Lyle; Oxford, Alexander William; Hynd, George; Archer, Janet Ann; Aley, Amanda; Harris, Neil Victor
PATENT ASSIGNEE(S): Pharmagene Laboratories Limited, UK
SOURCE: PCT Int. Appl., 173 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005012263	A1	20050210	WO 2004-GB3184	20040723
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2532505	A1	20050210	CA 2004-2532505	20040723
EP 1648876	A1	20060426	EP 2004-743517	20040723
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
JP 2006528617	T	20061221	JP 2006-520897	20040723
US 20090018150	A1	20090115	US 2006-564010	20060111

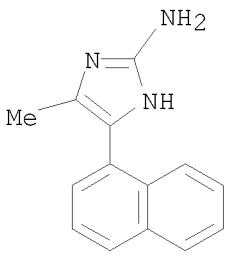
PRIORITY APPLN. INFO.:			
GB 2003-17346	A	20030724	
US 2003-490286P	P	20030728	
WO 2004-GB3184	W	20040723	

OTHER SOURCE(S): CASREACT 142:219297; MARPAT 142:219297

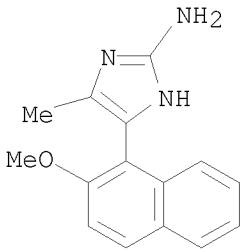
AB Title compds. represented by the formula I [wherein X = O or NH; R1 = (un)substituted aryl; R2, R3 = independently H, (un)substituted (cyclo)alkyl, cycloalkylalkyl, phenylalkyl; R4, R5 = independently H, (un)substituted (phenyl)alkyl, sulfonylalkyl, carbonylalkyl, alkylamino or R4R5 = (un)substituted heterocyclic group; and pharmaceutically acceptable salts or solvates thereof], and 3 addnl. Markush structures, were prepared as 5-HT2b receptor agonists. For example, reaction of 2-amino-4-chloro-6-methylpyrimidine with aniline in the microwave cavity gave II. I were tested for binding activity of 5-HT2A, 5-HT2B and 5-HT2C. Thus, I and their pharmaceutical compns. are useful for the treatment of a condition alleviated by antagonism of a 5-HT2B receptor, such as digestive tract disease (no data).

IT 842155-08-2P 842155-11-7P 842155-12-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinyl, imidazolyl, oxazolyl and triazolyl amine derivs. as 5-HT2b receptor antagonists)

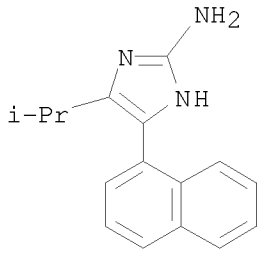
RN 842155-08-2 CAPLUS
CN 1H-Imidazol-2-amine, 4-methyl-5-(1-naphthalenyl)- (CA INDEX NAME)



RN 842155-11-7 CAPLUS
CN 1H-Imidazol-2-amine, 5-(2-methoxy-1-naphthalenyl)-4-methyl- (CA INDEX NAME)



RN 842155-12-8 CAPLUS
CN 1H-Imidazol-2-amine, 4-(1-methylethyl)-5-(1-naphthalenyl)- (CA INDEX NAME)



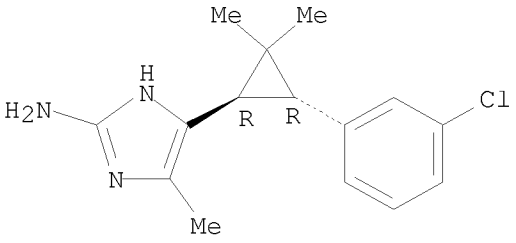
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:981473 CAPLUS
DOCUMENT NUMBER: 140:217525
TITLE: Aminoimidazoles as bioisosteres of acylguanidines: novel, potent, selective and orally bioavailable inhibitors of the sodium hydrogen exchanger isoform-1
AUTHOR(S): Ahmad, Saleem; Ngu, Khehyong; Combs, Donald W.; Wu, Shung C.; Weinstein, David S.; Liu, Wen; Chen, Bang-Chi; Chandrasena, Gamini; Dorso, Charles R.; Kirby, Mark; Atwal, Karnail S.
CORPORATE SOURCE: Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ, 08543, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(1), 177-180
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:217525
AB Inhibition of the sodium hydrogen exchanger isoform-1 (NHE-1) has been shown to limit damage to the myocardium under ischemic conditions in animals. While most known NHE-1 inhibitors are acylguanidines, this report describes the design and synthesis of a series of heterocyclic inhibitors of NHE-1 including aminoimidazoles with undiminished in vitro activity and oral bioavailability.
IT 335060-84-9P 335060-92-9P 665004-24-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of aminoimidazoles and related heterocyclic compds. as bioisosteres of acylguanidines and as inhibitors of the sodium hydrogen exchanger isoform-1)

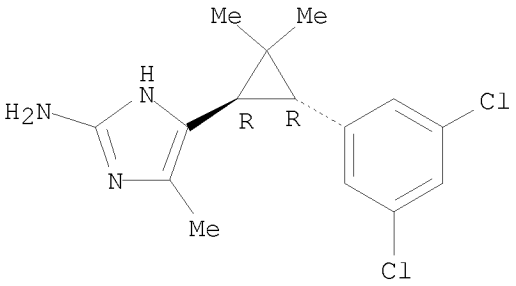
RN 335060-84-9 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3-chlorophenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



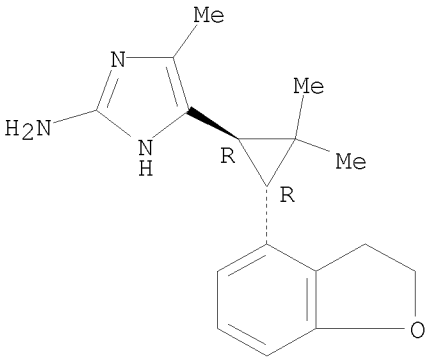
RN 335060-92-9 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3,5-dichlorophenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 665004-24-0 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(2,3-dihydro-4-benzofuranyl)-2,2-dimethylcyclopropyl]-4-methyl- (CA INDEX NAME)

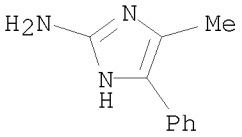
Absolute stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:855867 CAPLUS
DOCUMENT NUMBER: 139:214346
TITLE: Product class 3: imidazoles
AUTHOR(S): Grimmett, M. R.
CORPORATE SOURCE: Organic Chemistry, Dept. of Chemistry, University of Otago, Dunedin, N. Z.
SOURCE: Science of Synthesis (2002), 12, 325-528
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. Methods for preparing imidazoles are reviewed including cyclization, ring transformations, aromatization and modification of substituents on existing imidazoles.
IT 6646-81-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of imidazoles via cyclization, ring transformation, aromatization and substituent modifications)
RN 6646-81-7 CAPLUS
CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 823 THERE ARE 823 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2001:283949 CAPLUS
DOCUMENT NUMBER: 134:311218
TITLE: Synthesis and use of heterocyclic sodium/proton exchange inhibitors
INVENTOR(S): Ahmad, Saleem; Wu, Shung C.; O'Neil, Steven V.; Ngu, Khehyong; Atwal, Karnail S.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 221 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001027107	A2	20010419	WO 2000-US27461	20001002
WO 2001027107	A3	20020124		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 6887870	B1	20050503	US 2000-669298		20000925
CA 2388813	A1	20010419	CA 2000-2388813		20001002
EP 1224183	A2	20020724	EP 2000-968723		20001002
EP 1224183	B1	20051228			

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL

BR 2000014725	A	20030617	BR 2000-14725		20001002
HU 2003000195	A2	20030728	HU 2003-195		20001002
HU 2003000195	A3	20030929			
JP 2003527331	T	20030916	JP 2001-530325		20001002
NZ 517668	A	20040924	NZ 2000-517668		20001002
AT 314364	T	20060115	AT 2000-968723		20001002
ES 2254236	T3	20060616	ES 2000-968723		20001002
IN 2002MN00354	A	20050318	IN 2002-MN354		20020322
ZA 2002002479	A	20040727	ZA 2002-2479		20020327
MX 2002003626	A	20030922	MX 2002-3626		20020410
US 20050137216	A1	20050623	US 2005-46993		20050131
US 7326705	B2	20080205			

PRIORITY APPLN. INFO.:	US 1999-158755P	P	19991012
	US 2000-669298	A3	20000925
	WO 2000-US27461	W	20001002

OTHER SOURCE(S): MARPAT 134:311218

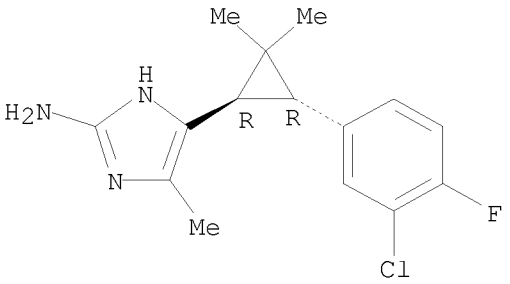
AB Compds. of formula I [wherein; n is 1-5; X is N or CR5, where R5 is H, halo, alkenyl, alkynyl, alkoxy, alkyl, aryl or heteroaryl; Z is a heteroaryl group; R1 is H, alk(en)(yn)yl, alk(enyl)(ynyl)oxy, (aryl or alkyl)3Si, cycloalk(en)yl, (aryl)amino, aryl(alkyl), cycloheteroaryl, etc.; R2, R3 and R4 are any of the groups set out for R1 and optionally substituted with 1 to 5 substituents which may be the same or different and when X is N, R1 is preferably aryl or heteroaryl] are claimed. Several hundred examples are disclosed. Synthesis of II proceeds via cyclopropanation of the cinnamate derived from the olefination between 3,5-dichlorobenzaldehyde and t-butyldiethylphosphonoacetate. The intermediate tert-Bu ester is converted to the corresponding α-chloroketone and reacted with acetyl guanidine to provide II in a total of 5 steps. Compds. I are said to be sodium/proton exchange inhibitors (NHE). Pharmaceutical combinations are claimed using I and certain antihypertensive agents, β-adrenergic agonists, hypolipidemic agents, antidiabetic agents, antiobesity agents, etc. Compds. I are useful as antianginal and cardioprotective agents and provide a method for preventing or treating angina pectoris, cardiac dysfunction, myocardial necrosis, and arrhythmia.

IT 335060-95-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(synthesis and use of heterocyclic sodium/proton exchange inhibitors)

RN 335060-95-2 CAPLUS

CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3-chloro-4-fluorophenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.

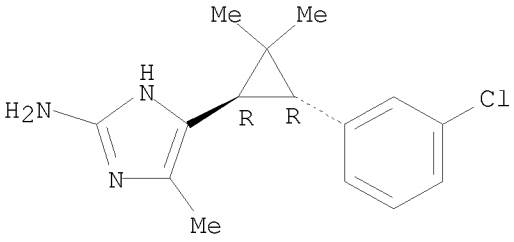


IT 335060-84-9P 335060-88-3P 335060-92-9P
335060-98-5P 335060-99-6P 335061-38-6P
335061-39-7P 335061-40-0P 335061-41-1P
335061-42-2P 335061-43-3P 335061-46-6P
335061-47-7P 335061-62-6P 335061-63-7P
335061-64-8P 335061-68-2P 335061-71-7P
335061-73-9P 335061-74-0P 335061-75-1P
335061-76-2P 335061-77-3P 335061-78-4P
335061-79-5P 335061-83-1P 335061-84-2P
335061-99-9P 335062-00-5P 335062-01-6P
335062-02-7P 335062-03-8P 335062-04-9P
335062-05-0P 335062-06-1P 335064-98-7P
335065-00-4P 335065-02-6P 335065-04-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and use of heterocyclic sodium/proton exchange inhibitors)

RN 335060-84-9 CAPLUS

CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3-chlorophenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

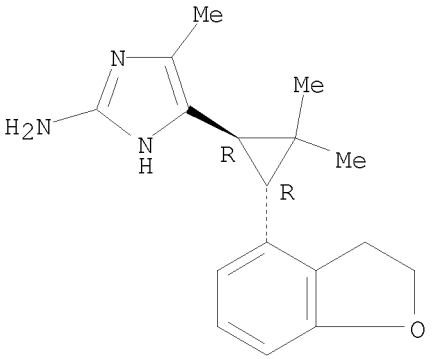
Relative stereochemistry.



RN 335060-88-3 CAPLUS

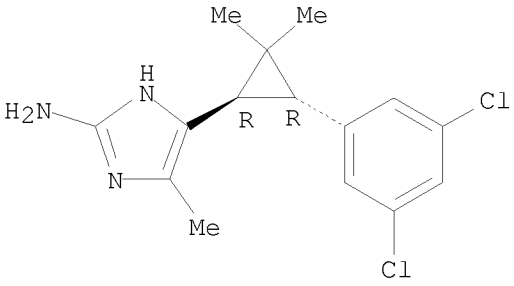
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(2,3-dihydro-4-benzofuranyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



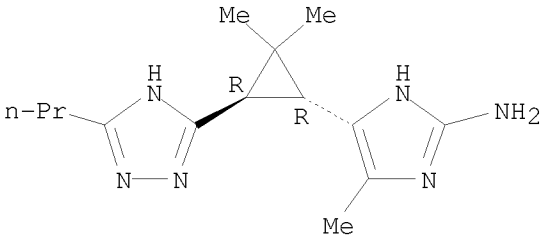
RN 335060-92-9 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3,5-dichlorophenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 335060-98-5 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-2,2-dimethyl-3-(3-propyl-1H-1,2,4-triazol-5-yl)cyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.

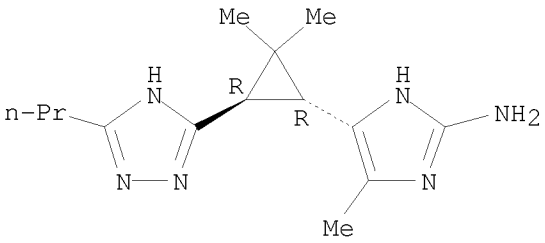


RN 335060-99-6 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-2,2-dimethyl-3-(3-propyl-1H-1,2,4-triazol-5-yl)cyclopropyl]-4-methyl-, rel-, 2,2,2-trifluoroacetate (1:?) (CA INDEX NAME)

CM 1

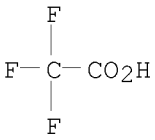
CRN 335060-98-5
CMF C14 H22 N6

Relative stereochemistry.



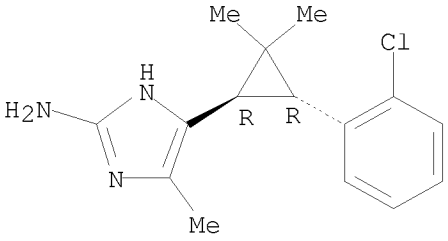
CM 2

CRN 76-05-1
CMF C2 H F3 O2



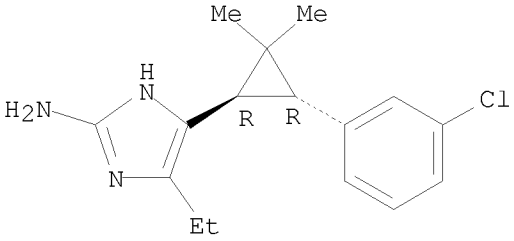
RN 335061-38-6 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(2-chlorophenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



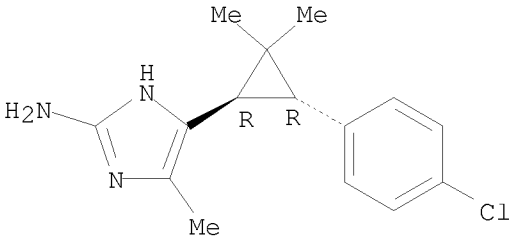
RN 335061-39-7 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3-chlorophenyl)-2,2-dimethylcyclopropyl]-4-ethyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



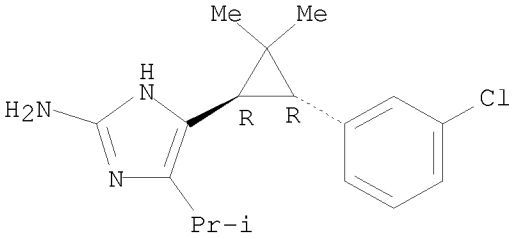
RN 335061-40-0 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(4-chlorophenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



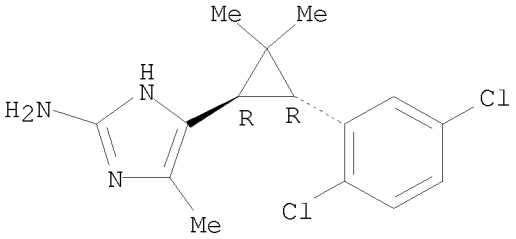
RN 335061-41-1 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3-chlorophenyl)-2,2-dimethylcyclopropyl]-4-(1-methylethyl)-, rel- (CA INDEX NAME)

Relative stereochemistry.



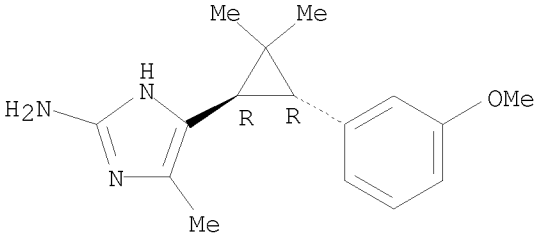
RN 335061-42-2 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(2,5-dichlorophenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 335061-43-3 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3-methoxyphenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

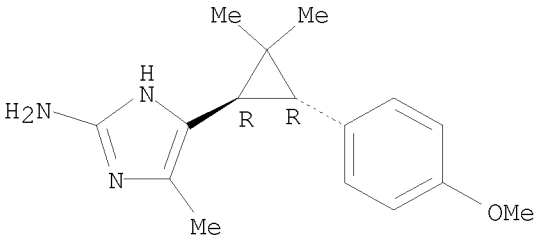
Relative stereochemistry.



RN 335061-46-6 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(4-methoxyphenyl)-2,2-

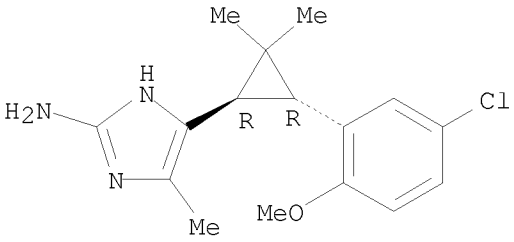
dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



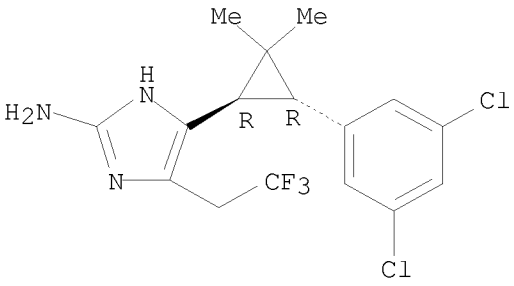
RN 335061-47-7 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(5-chloro-2-methoxyphenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



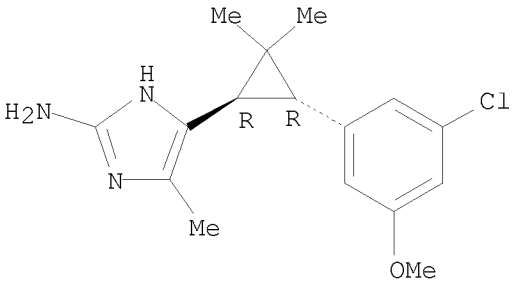
RN 335061-62-6 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3,5-dichlorophenyl)-2,2-dimethylcyclopropyl]-4-(2,2,2-trifluoroethyl)-, rel- (CA INDEX NAME)

Relative stereochemistry.



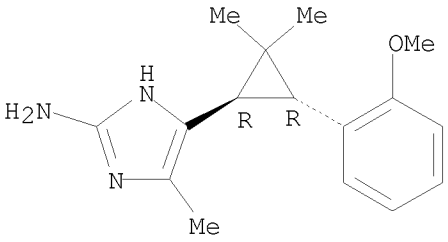
RN 335061-63-7 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3-chloro-5-methoxyphenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



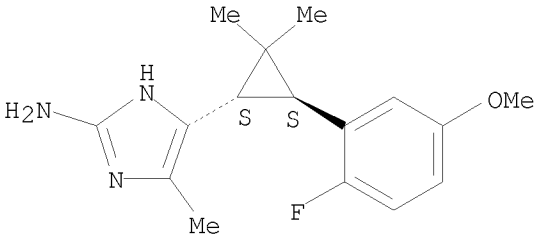
RN 335061-64-8 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(2-methoxyphenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



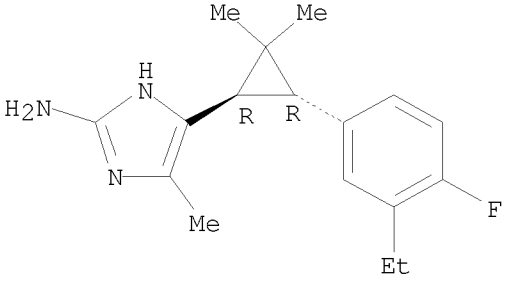
RN 335061-68-2 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(2-fluoro-5-methoxyphenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



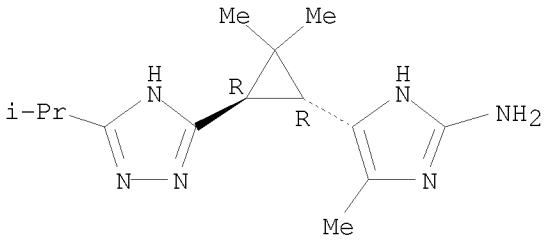
RN 335061-71-7 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3-ethyl-4-fluorophenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



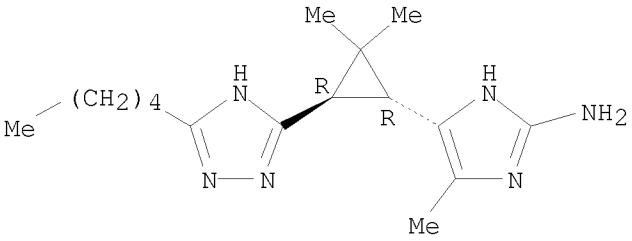
RN 335061-73-9 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-2,2-dimethyl-3-[3-(1-methylethyl)-1H-1,2,4-triazol-5-yl]cyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



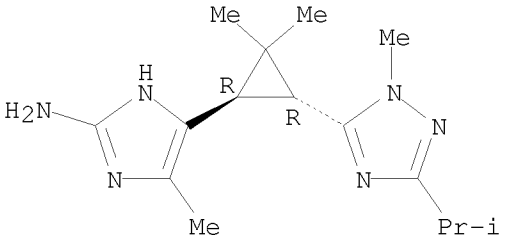
RN 335061-74-0 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-2,2-dimethyl-3-(3-pentyl-1H-1,2,4-triazol-5-yl)cyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



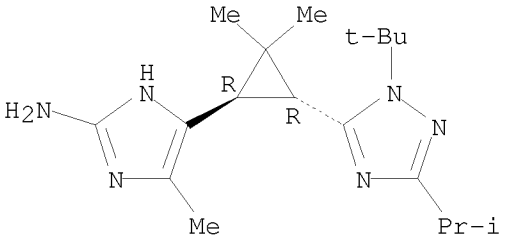
RN 335061-75-1 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-2,2-dimethyl-3-[1-methyl-3-(1-methylethyl)-1H-1,2,4-triazol-5-yl]cyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



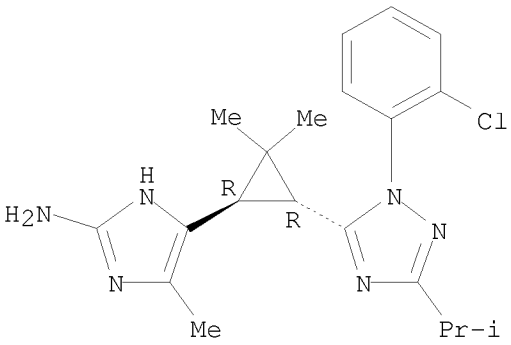
RN 335061-76-2 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-[1-(1,1-dimethylethyl)-3-(1-methylethyl)-1H-1,2,4-triazol-5-yl]-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



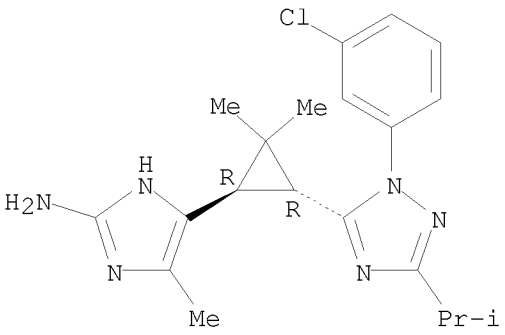
RN 335061-77-3 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-[1-(2-chlorophenyl)-3-(1-methylethyl)-1H-1,2,4-triazol-5-yl]-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



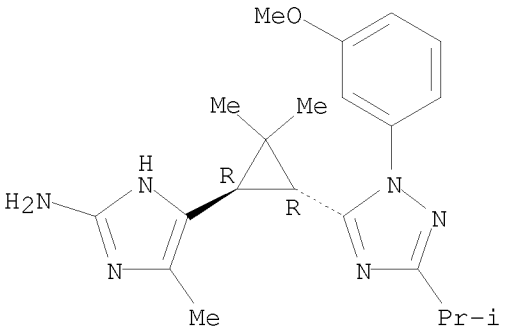
RN 335061-78-4 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-[1-(3-chlorophenyl)-3-(1-methylethyl)-1H-1,2,4-triazol-5-yl]-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



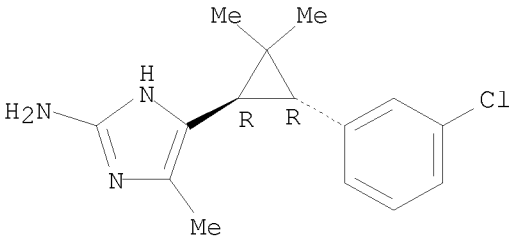
RN 335061-79-5 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-[1-(3-methoxyphenyl)-3-(1-methylethyl)-1H-1,2,4-triazol-5-yl]-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



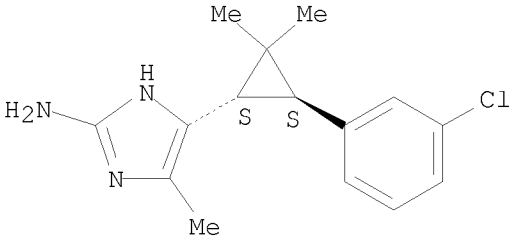
RN 335061-83-1 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3-chlorophenyl)-2,2-dimethylcyclopropyl]-4-methyl- (CA INDEX NAME)

Absolute stereochemistry.



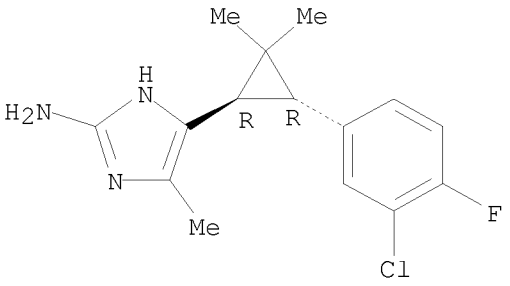
RN 335061-84-2 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1S,3S)-3-(3-chlorophenyl)-2,2-dimethylcyclopropyl]-4-methyl- (CA INDEX NAME)

Absolute stereochemistry.



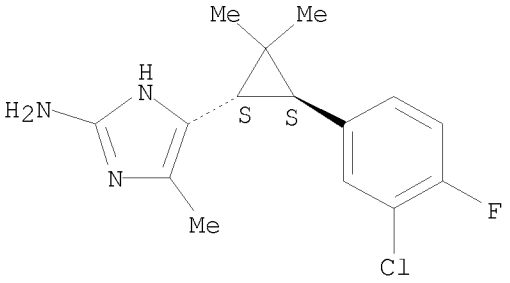
RN 335061-99-9 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3-chloro-4-fluorophenyl)-2,2-dimethylcyclopropyl]-4-methyl- (CA INDEX NAME)

Absolute stereochemistry.



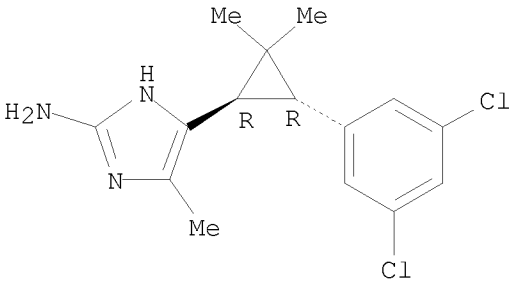
RN 335062-00-5 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1S,3S)-3-(3-chloro-4-fluorophenyl)-2,2-dimethylcyclopropyl]-4-methyl- (CA INDEX NAME)

Absolute stereochemistry.



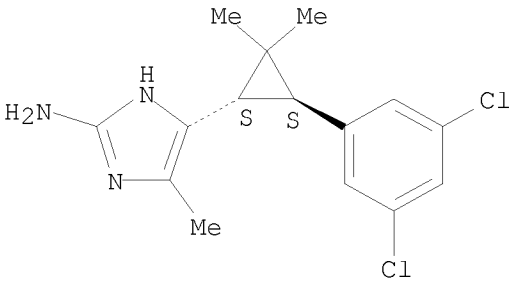
RN 335062-01-6 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3,5-dichlorophenyl)-2,2-dimethylcyclopropyl]-4-methyl- (CA INDEX NAME)

Absolute stereochemistry.



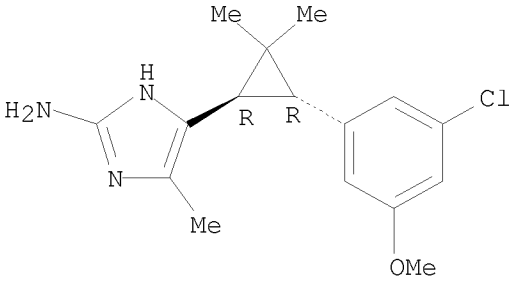
RN 335062-02-7 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1S,3S)-3-(3,5-dichlorophenyl)-2,2-dimethylcyclopropyl]-4-methyl- (CA INDEX NAME)

Absolute stereochemistry.



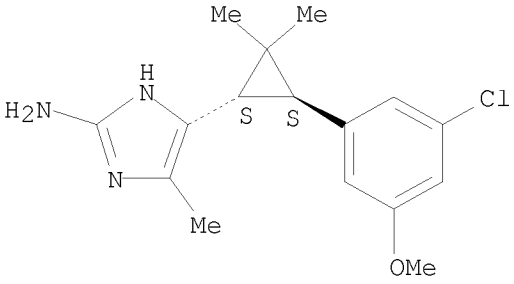
RN 335062-03-8 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(3-chloro-5-methoxyphenyl)-2,2-dimethylcyclopropyl]-4-methyl- (CA INDEX NAME)

Absolute stereochemistry.



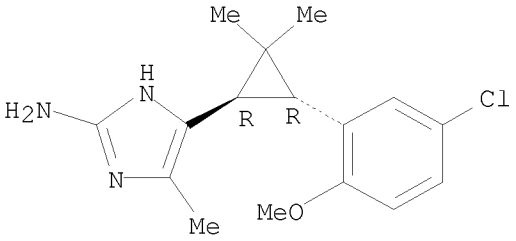
RN 335062-04-9 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1S,3S)-3-(3-chloro-5-methoxyphenyl)-2,2-dimethylcyclopropyl]-4-methyl- (CA INDEX NAME)

Absolute stereochemistry.



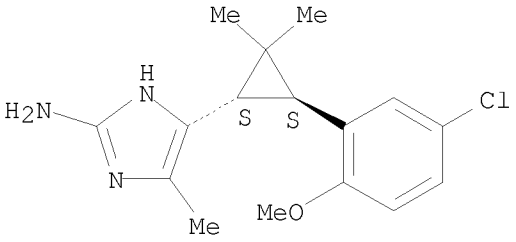
RN 335062-05-0 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(5-chloro-2-methoxyphenyl)-2,2-dimethylcyclopropyl]-4-methyl- (CA INDEX NAME)

Absolute stereochemistry.



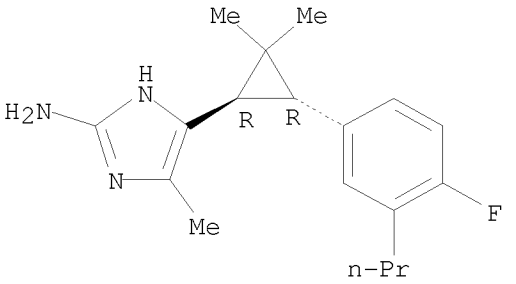
RN 335062-06-1 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1S,3S)-3-(5-chloro-2-methoxyphenyl)-2,2-dimethylcyclopropyl]-4-methyl- (CA INDEX NAME)

Absolute stereochemistry.



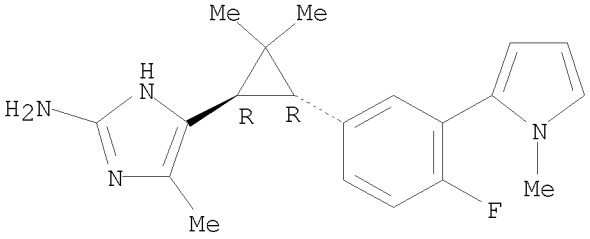
RN 335064-98-7 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(4-fluoro-3-propylphenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 335065-00-4 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-[4-fluoro-3-(1-methyl-1H-pyrrol-2-yl)phenyl]-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

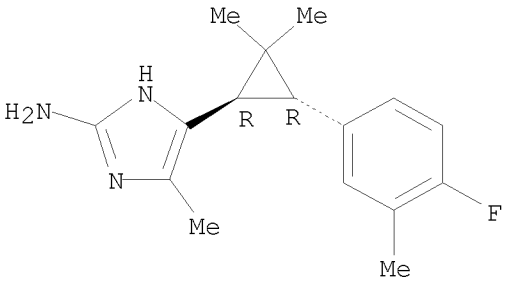
Relative stereochemistry.



RN 335065-02-6 CAPLUS

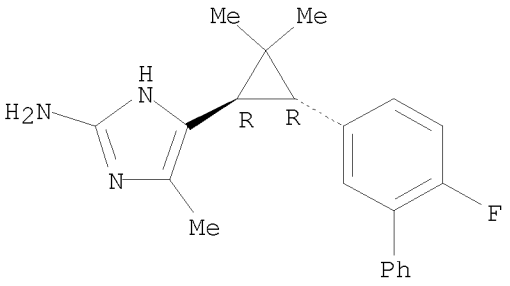
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(4-fluoro-3-methylphenyl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



RN 335065-04-8 CAPLUS
CN 1H-Imidazol-2-amine, 5-[(1R,3R)-3-(6-fluoro[1,1'-biphenyl]-3-yl)-2,2-dimethylcyclopropyl]-4-methyl-, rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2000:98527 CAPLUS
DOCUMENT NUMBER: 132:137388
TITLE: Preparation of N-imidazolylalkyl-2-imidazoleamines as histamine H3 receptor ligands
INVENTOR(S): Jegham, Samir; Saady, Mourad; Yaiche, Philippe; Horter, Laurence
PATENT ASSIGNEE(S): Sanofi-Synthelabo, Fr.
SOURCE: PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000006552	A1	20000210	WO 1999-FR1824	19990726

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

FR 2781798	A1	20000204	FR 1998-9602		19980728
FR 2781798	B1	20000908			
AU 9949166	A	20000221	AU 1999-49166		19990726
PRIORITY APPLN. INFO.:			FR 1998-9602	A	19980728
			WO 1999-FR1824	W	19990726

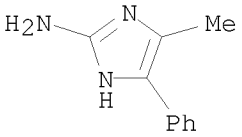
OTHER SOURCE(S): MARPAT 132:137388

AB RZNH(CH2)mR1 (R1 = 1H-imidazole-4-yl)[I; R = (un)substituted Ph; Z = (un)substituted 1H-imidazole-5,2-diyl; m = 2-4] were prepared Thus, PhCH(OH)COPh was cyclocondensed with urea and the chlorinated product aminated by H2CH2Ph to give, after deprotection, 4,5-diphenyl-1H-imidazole-2-amine which was amidated by 1H-imidazole-4-propanoic acid and the product reduced to give I (R = Ph, Z = 3-phenyl-1H-imidazole-5,2-diyl, m = 3). Data for biol. activity of I were given.

IT 6646-81-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of N-imidazolylalkyl-2-imidazoleamines as histamine H3 receptor ligands)

RN 6646-81-7 CAPLUS

CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1999:659664 CAPLUS

DOCUMENT NUMBER: 131:271809

TITLE: Preparation of 3-(α-heteroarylaminobenzylidene)-2-indolinones as Cyclin dependent kinase inhibitors

INVENTOR(S): Grell, Wolfgang; Walter, Rainer; Heckel, Armin; Himmelsbach, Frank; Wittneben, Helmut; van Meel, Jakobus; Redemann, Norbert; Haigh, Robert

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany

SOURCE: Ger. Offen., 64 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19815020	A1	19991007	DE 1998-19815020	19980403
US 6043254	A	20000328	US 1999-277063	19990326
WO 9951590	A1	19991014	WO 1999-EP2186	19990330

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ,

TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

AU 9937034	A	19991025	AU 1999-37034		19990330
PRIORITY APPLN. INFO.:			DE 1998-19815020	A	19980403
			US 1998-86733P	P	19980526
			WO 1999-EP2186	W	19990330

OTHER SOURCE(S): MARPAT 131:271809

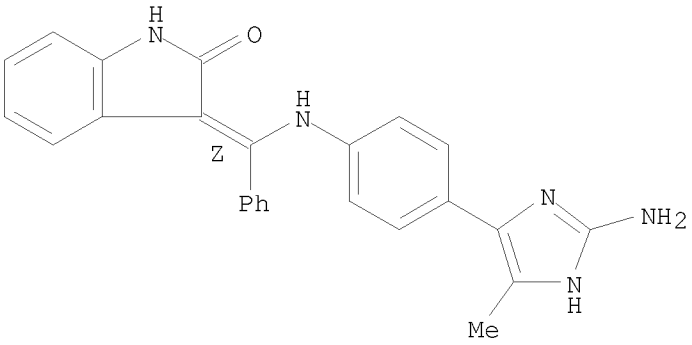
AB Title compds. [I; R = H; R1 = H, halo, NO2, (alkanoyl)amino, etc.; R2 = (un)substituted Ph; R4 = NHR3; R3 = heteroannelated Ph, heteroarylalk(en)ylphenyl, etc.] were prepared Thus,2-indolinone was N-acetylated and the product condensed with PhC(OEt)3 to give I (R1 = H, R2 = Ph)(II; R = Ac, R4 = OEt) which was condensed with 5-aminoindole to give II (R = H, R4 = 5-indolylamino). Data for biol. activity of I were given.

IT 1139222-15-3
RL: PRPH (Prophetic)
(Preparation of 3-(α-heteroarylaminobenzylidene)-2-indolinones as Cyclin dependent kinase inhibitors)

RN 1139222-15-3 CAPLUS

CN 2H-Indol-2-one, 3-[[[4-(2-amino-4-methyl-1H-imidazol-5-yl)phenyl]amino]phenylmethylene]-1,3-dihydro-, (3Z)- (CA INDEX NAME)

Double bond geometry as shown.

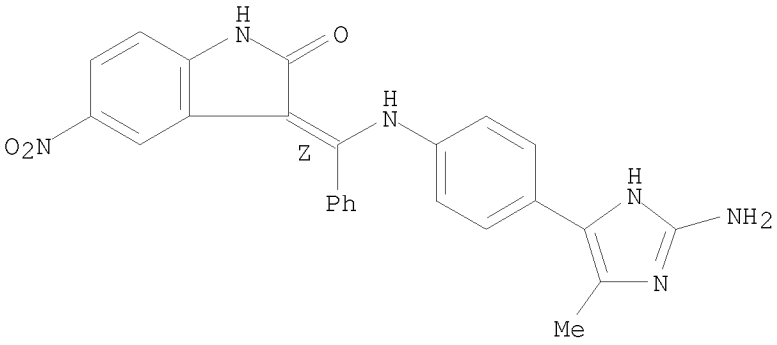


IT 245546-03-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3-(α-heteroarylaminobenzylidene)-2-indolinones as cyclin dependent kinase inhibitors)

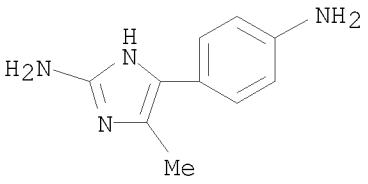
RN 245546-03-6 CAPLUS

CN 2H-Indol-2-one, 3-[[[4-(2-amino-4-methyl-1H-imidazol-5-yl)phenyl]amino]phenylmethylene]-1,3-dihydro-5-nitro-, (3Z)- (CA INDEX NAME)

Double bond geometry as shown.



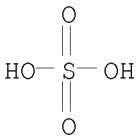
IT 245547-21-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 3-(α-heteroarylaminobenzylidene)-2-indolinones as cyclin dependent kinase inhibitors)
RN 245547-21-1 CAPLUS
CN 1H-Imidazol-2-amine, 5-(4-aminophenyl)-4-methyl- (CA INDEX NAME)



L10 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1995:183280 CAPLUS
DOCUMENT NUMBER: 122:55805
ORIGINAL REFERENCE NO.: 122:10814h,10815a
TITLE: A Simple and Practical Synthesis of 2-Aminoimidazoles
AUTHOR(S): Little, Thomas L.; Webber, Stephen E.
CORPORATE SOURCE: Agouron Pharmaceuticals Inc., San Diego, CA, 92121, USA
SOURCE: Journal of Organic Chemistry (1994), 59(24), 7299-305
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:55805
AB A new and simple two-step procedure to synthesize 2-aminoimidazoles (2-AI's) from readily available materials has been developed. The cyclization reaction of α-halo ketones RCOCHR1X [R = Me, Et, CMe3, Ph, 4-BrC6H4, etc., R1 = H, Me, Ph, RR1 = (CH2)3, (CH2)4, X = Cl, Br] and N-acetylguanidine in acetonitrile (MeCN) at reflux, or in DMF at ambient temperature, gives 4(5)-substituted and 4,5-disubstituted N-(1H-imidazol-2-yl)acetamides I, which are then hydrolyzed to their resp. 2-AI's. In general, the purified products were isolated in good yields. We have prepared several examples and have demonstrated the usefulness of this method by its application in the total synthesis of 2-aminohistamine, an interesting histamine analog, and oroidin (II), a marine natural product isolated from various sponges.
IT 6646-80-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 6646-80-6 CAPLUS
CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl-, sulfate (2:1) (CA INDEX NAME)

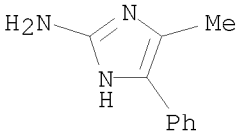
CM 1

CRN 7664-93-9
CMF H2 O4 S



CM 2

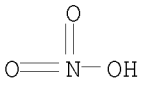
CRN 6646-81-7
CMF C10 H11 N3



L10 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1979:121484 CAPLUS
DOCUMENT NUMBER: 90:121484
ORIGINAL REFERENCE NO.: 90:19231a,19234a
TITLE: Reaction of guanidines with α-diketones. Syntheses of 4,5-disubstituted-2-aminoimidazoles and 2,6-unsymmetrically substituted imidazo[4,5-d]imidazoles
AUTHOR(S): Nishimura, Tamio; Kitajima, Koji
CORPORATE SOURCE: Sch. Hyg. Sci., Kitasato Univ., Sagamihara, Japan
SOURCE: Journal of Organic Chemistry (1979), 44(5), 818-24
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 90:121484
AB Cyclocondensation of RCOCOR1 (I; R = R1 = Ph, p-MeO2C6H4, p-ClC6H4, p-MeC6H4, Me; R = Me, R1 = Ph) with R22NC(:NH)NH2 (R2 = H, Me) in dioxane followed by hydrogenation over Pd/C gave 2-aminoimidazoles II via 4H-imidazol-4-ols III. However, similar treatment of I (R = R1 = Ph) with 1-amidino-3,5-dimethylpyrazole gave imidazoimidazole IV instead of the expected V.
IT 68212-73-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 68212-73-7 CAPLUS
CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl-, nitrate (1:1) (CA INDEX NAME)

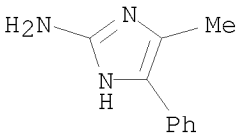
CM 1

CRN 7697-37-2
CMF H N O3



CM 2

CRN 6646-81-7
CMF C10 H11 N3



L10 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1969:47448 CAPLUS
DOCUMENT NUMBER: 70:47448
ORIGINAL REFERENCE NO.: 70:8914h,8915a
TITLE: 2-Aminoimidazole derivatives
INVENTOR(S): Lancini, Giancarlo; Lazzari, Ettore
PATENT ASSIGNEE(S): Lepetit S.p.A.
SOURCE: Brit., 4 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1132013		19681030	GB 1965-16050	19650414

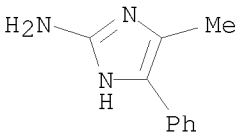
AB I, where R, R1, and R2 are H, alkyl, aryl, or aralkyl, are prepared by the reaction of R1COCHR2NHR with H2NCN in H2O solution at 70-100° 0.5-1.5 hrs. at pH 3-7 when R1 is H, or pH 4-5 when R1 is alkyl, etc. Thus, a solution of 5 g. MeCOCH2NH2. HCl and 5 g. H2NCN in 30 ml. H2O was adjusted to pH 6 with NaOH, then pH 4.5 with HOAc. The solution was heated to 85-95° 45 min. to give 82% I (R = R2 = H, R1 = Me).HCl, m. 115-17° (Et2O-EtOH); picrate m. 186-7°. Other I similarly were prepared (R, R1, R2, m.p. HCl salt, and m.p. of picrate given): H, Me, Me, 289°, -; H, Me, PhCH2, 159-60°, -; H, Ph, H, 207-9°, 227-8°; H, Me, Ph, 84-5°, 214-17°; Me, Ph, H, 125-7°, 247-9°. To a solution of 4.6 g. Et sarcosinate-HCl in 35 ml. H2O were added 200 g. of 2.5% Na/ Hg over 1 hr., the mixture being kept acid with HCl at -5° to 0°, by addition of solid CO2. After 30 min. at 0° the Hg was removed and the solution of MeNHCH2CHO added with 3.5 g. H2NCN at pH 4.5 on a steam bath and left 1 hr. to give a residue which was extracted with Et2O, dissolved in a small volume H2O, and added to a boiling solution of picric acid in H2O to give 2.2 g. I (R = Me, R1 = R2 = H) picrate, m. 208-10°. Other I similarly prepared were (R, R1, R2, and HCl salt m.p. given): Me, H, Me, 257° (decomposition); Me, H, Et, 201-3°.

IT 6752-09-6P 21541-12-8P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)
RN 6752-09-6 CAPLUS
CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl-, compd. with 2,4,6-trinitrophenol (1:?) (CA INDEX NAME)

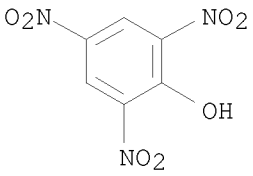
CM 1

CRN 6646-81-7
CMF C10 H11 N3

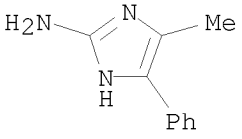


CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



RN 21541-12-8 CAPLUS
CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

L10 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1967:76011 CAPLUS
DOCUMENT NUMBER: 66:76011
ORIGINAL REFERENCE NO.: 66:14263a,14266a
TITLE: 2-Aminoimidazoles
PATENT ASSIGNEE(S): Lepetit S.p.A.
SOURCE: Neth. Appl., 7 pp.
CODEN: NAXXAN
DOCUMENT TYPE: Patent
LANGUAGE:
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6604949		19661017	NL 1966-4949	19660413
DE 1595899			DE	
FR 1475415			FR	
GB 1132013			GB	
US 3450709		19690617	US	19660328

PRIORITY APPLN. INFO.: GB 19650414

AB The title compds. of the general formula I were prepared by treating the corresponding R1COCHR2NHR with excess cyanamide (II) in water at a pH between 4.5 and 5 at 70-100°. Thus, 200 g. 2.5% Na amalgam was added in 1 hr. to a solution of 4.6 g. ethyl sarcosine hydrochloride in 35 cc. water in the presence of 15% HCl at -5 to 0°, the mixture stirred 30 min. at 0°, and the Hg discarded. II (3.5 g.) was added at a pH of 4.5, and the solution heated 1 hr. on a steam bath to yield I (R1 and R2 = H, R = Me); picrate m. 208-10°; HCl salt m. 84-5°. Similarly prepared were I (R, R1, R2, m.p. HCl salt, and m.p. picrate given): Me, H, Me, 257° (decomposition), -; Me, H, Et, 201-3° -; H, Me, Me, 289° -; H, Me, H, 115-17°, 186-7°; H, Me, benzyl, 159-60°, -; H, Ph, H, 207-9°, 227-8°; H, Me, Ph, 84-5°, 214-17°; Me, Ph, H, 125-7°, 247-9°. I are used as intermediates for preparing azomycin and its homologs and analogs.

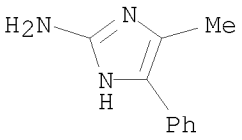
IT 6752-09-6P 13805-36-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 6752-09-6 CAPLUS

CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl-, compd. with 2,4,6-trinitrophenol (1:?) (CA INDEX NAME)

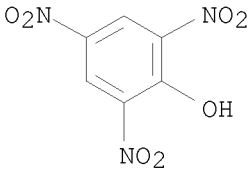
CM 1

CRN 6646-81-7
CMF C10 H11 N3



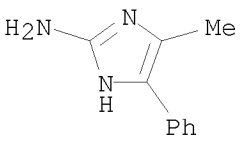
CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



RN 13805-36-2 CAPLUS

CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl-, hydrochloride (1:?) (CA INDEX NAME)

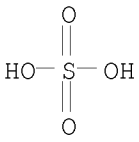


●x HCl

L10 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1966:420794 CAPLUS
DOCUMENT NUMBER: 65:20794
ORIGINAL REFERENCE NO.: 65:3857g-h
TITLE: A new synthesis of alkyl and aryl 2-aminoimidazoles
AUTHOR(S): Lancini, Gian Carlo; Lazzari, Ettore
SOURCE: Journal of Heterocyclic Chemistry (1966), 3(2), 152-4
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 65:20794
AB The condensation of cyanamide with α-aminocarbonyl compds. has been studied as a method of synthesizing alkyl and aryl 2-aminoimidazoles. Starting from Nalkylaminoaldehydes, 1,5-dialkyl-2-aminoimidazoles have been prepared Starting from suitable aminoketones a variety of monosubstituted and disubstituted derivs. was obtained.
IT 6646-80-6 6646-81-7 6752-09-6
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 6646-80-6 CAPLUS
CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl-, sulfate (2:1) (CA INDEX NAME)

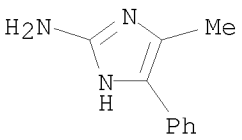
CM 1

CRN 7664-93-9
CMF H2 O4 S

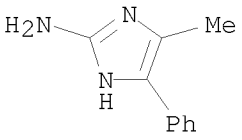


CM 2

CRN 6646-81-7
CMF C10 H11 N3



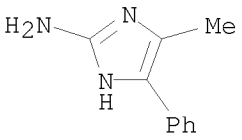
RN 6646-81-7 CAPLUS
CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl- (CA INDEX NAME)



RN 6752-09-6 CAPLUS
CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl-, compd. with 2,4,6-trinitrophenol (1:?) (CA INDEX NAME)

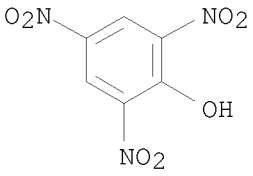
CM 1

CRN 6646-81-7
CMF C10 H11 N3



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



L10 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1966:420793 CAPLUS
DOCUMENT NUMBER: 65:20793
ORIGINAL REFERENCE NO.: 65:3857c-g
TITLE: Synthesis and conversions of 2-formylbenzimidazoles
AUTHOR(S): Dalgatov, D. D.
SOURCE: Sb. Aspirantskikh Rabot, Dagestansk. Univ., Estestv, i Fiz.-Mat. Nauk, Makhachkala (1964) 69-75
From: Ref. Zh., Khim. 1966(4), Pt. I, Abstr. No. 4Zh317.

DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB Methods for synthesis of 2-formylbenzimidazoles (I) and the N-Me (II) and N-Ph (III) derivs. of I were studied. II was condensed with Me ketones and $PhCH_2NO_2$ (IV) and I and II were condensed with cyclohexanone (V). 1,2-Bis(2-benzimidazolyl)ethylene glycol (2.94 g.) was dissolved in 100 ml. N HCl, 2.3 g. KIO_4 added, the solution kept 2 days at 20°, and 10% Na_2CO_3 added to alkalinity to yield 93% I, m. 235° (alc.) (decomposition). I (1.46 g.), 7 ml. V, and 7 ml. MeOH was heated at 100°, 5-6 drops 20% KOH added, and the mixture cooled after 10-15 min. to yield 75% the 2-(2-benzimidazolylmethylene) derivative of V, sublimes 175-80° (MeOH). KOH (5.6 g.) and 13.2 g. 2-methylbenzimidazole (VI) in 50 ml. alc. was boiled, 17.2 g. $PhSO_3Me$ added after 1 hr., the mixture heated 2 hrs. and filtered, and the filtrate evaporated to give 10.3 g. 1-Me derivative (VIa) of VI, m. 112° (H_2O). Oxidation of VIa with SeO_2 in PhMe at 95° yielded 40% II. 1-Methyl-2-(hydroxymethyl)benzimidazole (1.6 g.) was dissolved in 50 ml. 2N H_2SO_4, 0.05 g. $AgNO_3$ added, the mixture heated to 70° $K_2S_2O_8$ added after 4 hrs., the mixture filtered, and the filtrate neutralized with Na_2CO_3 solution to yield 0.4 g. II, m. 110°. II (1.6 g.) and 1.49 g. isonicotinic hydrazide in 8 ml. MeOH was boiled 20 min. to yield 2 g. isonicotinoyl hydrazone of II, m. 200-3° (MeOH). 2-(Hydroxymethyl)benzimidazole (VII) (14.8 g.), 21.2 g. unsatd. leukotrone O, and a concentrated solution of 4 g. NaOH was heated 4 hrs., and Me_2NPh steam distilled to yield 12 g. 1-$PhCH_2$ derivative of VII, m. 186.5-87° (alc.). To 1.6 g. II and 1.99 g. p-bromoacetophenone (VIII) in 3 ml. MeOH was added 2-3 drops 5% KOH to yield 70% 2-[β-(p-bromobenzoyl)vinyl]-1-methylbenzimidazole, m. 159-60° (alc.). II (1.6 g.) and 3.98 g. VIII were dissolved in 10 ml. hot MeOH, 2 ml. 20% KOH added, and the mixture boiled 1 hr. to yield 74% 1-methyl-2-bis(p-bromo-phenacylmethyl)benzimidazole, m. 186.5-87° (MeOH). Analogously was obtained 2-(β-tolylvinyl)-1-methylbenzimidazole, m. 134° (alc.). II (1.6 g.) and 0.98 g. IV in 5 ml. MeOH and 3 drops 10% KOH was boiled 0.5 hr. to yield 1.7 g. 2-(1-methyl-2-benzimidazolylmethylene) derivative of V, m. 237° ($CHCl_3$). To 1.37 g. IV in 8 ml. alc. was added 1 g. NaOH in 8 ml. H_2O and in portions 1.6 g. of a solution of II in 10 ml. alc. and after 5 hrs. the mixture neutralized with 1:1 aqueous HCl to yield 73% 2-(β-nitro-α-hydroxy-β-phenylethyl)-1-methylbenzimidazole, m. 162-3° (decomposition) (alc.-Me_2CO). To 20.8 g. 2-methyl-1-phenylbenzimidazole in 200 ml. anhydrous PhMe at 95° was added 11.1 g. SeO_2 over 4 hrs., the mixture heated 2 hrs., the PhMe layer separated and steam distilled, and the residue treated with $CHCl_3$ to yield 35% III (oil); dinitrophenylhydrazone m. 260-1°; semi-carbazone m. 255-6°.

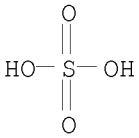
IT 6646-80-6 6646-81-7 6752-09-6
(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 6646-80-6 CAPLUS

CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl-, sulfate (2:1) (CA INDEX NAME)

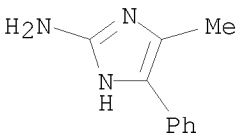
CM 1

CRN 7664-93-9
CMF H2 O4 S

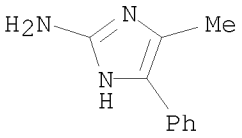


CM 2

CRN 6646-81-7
CMF C10 H11 N3



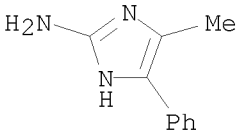
RN 6646-81-7 CAPLUS
CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl- (CA INDEX NAME)



RN 6752-09-6 CAPLUS
CN 1H-Imidazol-2-amine, 4-methyl-5-phenyl-, compd. with 2,4,6-trinitrophenol (1:?) (CA INDEX NAME)

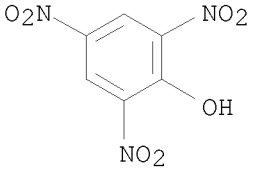
CM 1

CRN 6646-81-7
CMF C10 H11 N3



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



L10 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1963:469114 CAPLUS
DOCUMENT NUMBER: 59:69114

ORIGINAL REFERENCE NO.: 59:12784a-h
TITLE: Guanidino β-diketones. I. Synthesis and properties of some amino- and guanidino β-diketones with the β-diketone groups in the open chain
AUTHOR(S): Grinsteins, V.; Veveris, A.
SOURCE: Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija (1962), (No. 3), 463-71
CODEN: LZAKAM; ISSN: 0002-3248
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 59, 11363g. A solution of 3.5 g. isonitrosoacetylacetone in 30 ml. absolute alc. and 30 ml. 30% alc. HCl added to a catalyst (0.1 g. PtO_2 and 5 ml. alc. shaken 10 min. in H atmospheric) and the mixture hydrogenated 1.5-2 hrs., heated to boiling, and filtered cold gave 2.5 g. $AcCH(NH_2.HCl)Ac$ (I), m. 185-7° (decomposition). Similarly, $PhCH(OH)CH(NH_2.HCl)Ac$, m. 166-7° (decomposition) [p-nitrophenylhydrazone m. 196-7° (decomposition)], was obtained (62.5% yield) from BzC(:NOH)Ac. I (0.1 g.) in 0.5 g. H_2O heated with 0.1 ml. $N_2H_4.H_2O$ gave 0.045 g. 3,5-dimethyl-4-aminopyrazole, m. 203 5° (PrOH-petr. ether). $NaHCO_3$ (0.12 g.) added to a solution of 0.2 g. I in 2 ml. H_2O, the mixture kept 2 hrs., and the precipitate filtered off, dried, and extracted with petr. ether gave 0.11 g. 2,5-dimethyl-3,6-diacetylpyrazine, m. 97-9°. Isonitrosobenzoylacetone (1 g.) added portionwise during 1.5 hrs. to a solution of 2 ml. concentrated HCl, 2 ml. 20% alc. HCl, and 1.3 g. Pb powder, the mixture kept 20 min. at 40°, then 20 ml. 50% alc. and H_2S added, the precipitate filtered off, and the filtrate evaporated at 30-40° in vacuo gave 0.5 g. $BzCH(NH_2.HCl)Ac$ (II), m. 133-5° (decomposition) [alc.-AcOEt (1:10)]. p-Nitrobenzoylacetone (1 g.) in 20 ml. 3% KOH added at 40° to a solution obtained from 13.4 g. $FeSO_4$ dissolved in 25 ml. hot H_2O and mixed with 7 g. KOH in 10 ml. H_2O, the mixture kept 20 min. at 20°, cooled to 0° and filtered, the filtrate acidified with AcOH, and kept 12 hrs. at 0°, precipitate filtered off gave 0.6 g. $p\text{-}H_2NC_6H_4COCH_2Ac$ (III), m. 93-5° (30 and 96% alc. consecutively). Similarly, from m-nitrobenzoylacetone was obtained 53.8% $m\text{-}H_2NC_6H_4$ analog, m. 72-4° [C_6H_6-petr. ether (1:1)]; hydrochloride m. 153-4° (decomposition). III (0.2 g.) in 1.5 ml. 15% KOH left for 3 days gave 0.11 g. p-aminoacetophenone, m. 104-6°. III (0.1 g.), 2 ml. C_6H_6, and 0.1 g. Ac_2O heated 15 min. on the steam bath and filtered cold gave 0.12 g. $p\text{-}AcNHC_6H_4COCH_2Ac$, m. 179-80° [alc.-$C_6H_6$ (1:4)]. Similarly were obtained $m\text{-}AcNHC_6H_4COCH_2Ac$, m. 101-2° (80.7% yield), and $m\text{-}AcNHC_6H_4COCH_2Bz$, m. 165-6° (alc.). p-Nitrodibenzoylmethane (2.1 g.), 2.7 g. Pb powder, 20 ml. alc., and 6 ml. concentrated HCl heated to 50° to dissolve Pb, 30 ml. alc. with 10 ml. H_2O added, the mixture saturated with H_2S, filtered, the filtrate treated with excess dilute NH_4OH, filtered, the residue on filtration dissolved in 20 ml. hot alc. and precipitated with 25 ml. hot H_2O gave 0.3 g. $p\text{-}H_2NC_6H_4COCH_2Bz$ (IV), m. 120-1° [C_6H_6-petr. ether (1:1)]; hydrochloride m. 187° (decomposition). Similarly was reduced m-nitrodibenzoylmethane; its amine, m. 86-7° (dilute alc.), dissolved in alc., treated with 27% alc. HCl, and precipitated with ether yielded 17.6% $m\text{-}H_2NC_6H_4COCH_2Bz.HCl$ (V), m. 198° (decomposition). p-Nitrobenzylacetylacetone (0.7 g.), 70 ml. absolute AcOEt, and 0.05 g. PtO_2 shaken 1 hr. in H atmospheric, filtered, and the filtrate treated with 0.5 ml. 30% alc. HCl gave 0.25 g. $p\text{-}H_2NC_6H_4CH_2CHAc_2.HCl$, m. 138-40° (decomposition) (PrOH). Similarly was obtained 23% yield $m\text{-}H_2NC_6H_4CHAc_2.HCl$, m. 136-8° (decomposition)(PrOH-AcOEt). I (0.3 g.) and 0.3 g. $NCNH_2$

heated 1.5 min. on a steam bath, 5 ml. 14% alc. HCl added, and the mixture heated 5 min. and filtered cold gave 0.2 g. VI, m. 255-60° (decomposition) (95% alc.); free amine m. 224-6° (decomposition) (alc.); thiosemicarbazone m. 267-8° (decomposition) (alc.). II (0.35 g.) and 0.35 g. NCNH2 heated 2-3 min. on the steam bath, 3 ml. 27% alc. HCl added, the mixture evaporated to dryness, 3 ml. H2O and 0.5 ml. concentrated HNO3 added, and the mixture left 15 min. gave 0.15 g. C11H11ON3.HNO3, m. 204° (decomposition) (H2O). V (0.25 g.), 0.1 g. NCNH2, and 2 ml. absolute alc. boiled 3 hrs., alc. distilled in vacuo, and the residue dissolved in H2O and treated with excess 2N HNO3 gave 0.15 g. m-H2NC(:NH)NHC6H4COCH2Bz.HNO3 (VII), m. 198° (decomposition). IV (0.4 g.) melted with 0.4 g. NCNH2, 0.6 ml. 27% absolute alc. HCl added, the mixture heated 7 min., 1.2 ml. addnl. acid added, and the mixture heated 7 min., poured in H2O, and precipitated with dilute NH4OH gave VII free amine, which, dissolved in 5 ml. 5% AcOH and 1 g. NaNO3, gave 0.5 g. p-analog of VII, m. 198-9° (decomposition) (H2O).

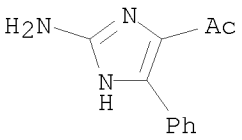
IT 96776-18-0
(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 96776-18-0 CAPLUS

CN Ethanone, 1-(2-amino-4-phenyl-1H-imidazol-5-yl)-, nitrate (1:1) (CA INDEX NAME)

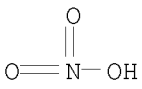
CM 1

CRN 96776-17-9
CMF C11 H11 N3 O



CM 2

CRN 7697-37-2
CMF H N O3



L10 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1963:469113 CAPLUS
DOCUMENT NUMBER: 59:69113
ORIGINAL REFERENCE NO.: 59:12783f-h,12784a
TITLE: Organic sulfonic acids. IX. Reactions of sultones with 1-phenyl-3-methyl-5-pyrazolone
AUTHOR(S): Helberger, Johann H.; Sproviero, Jorge F.
CORPORATE SOURCE: Tech. Univ., Berlin
SOURCE: Justus Liebigs Annalen der Chemie (1963), 666, 78-80
CODEN: JLACBF; ISSN: 0075-4617
DOCUMENT TYPE: Journal

LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 59:69113

AB To 15.6 g. 1-phenyl-3-methyl-5-pyrazolone (I) in 30 cc. o-C6H4Cl2 (Ia) heated at 110° (oil bath) was added 11 g. molten 3-hydroxy-1-propanesulfonic acid sultone (II), heated 4 hrs. at 170-5°, the solvent decanted from an amorphous solid, the latter dissolved in a little EtOH, the solution cooled, and the precipitate (22.7 g.) recrystd. from 90% EtOH to give 2-(3-sulfopropyl) derivative (III) of I, m. 228-30° (chromatography on Dowex 50 with aqueous EtOH followed by elution with H2O). PhNHNH2 (20 g.) in Et2O treated with 22.4 g. molten II (after a brief time, the reaction became vigorous and required cooling), the amorphous precipitate dissolved in a little H2O, the solution extracted with Et2O, and concentrated deposited 9 g. PhNHNH(CH2)3SO3H, m. 221-2° (70% MeOH). III (36 g.) suspended in 70 cc. H2O treated with 11.4 cc. concentrated HCl and then with 9.6 g. NaNO2 (13% aqueous solution) at 0-5° with stirring (by testing with KI-starch paper, the NaNO2 addition was controlled so that no excess appeared), the resulting solid treated with 80 cc. ice cold EtOH, and filtered excluding direct sunlight gave 17 g. 4-NO derivative (IV) of III, pale yellow solid. IV (4.9 g.) in 80 cc. H2O treated 2 hrs. with a current of H2S (light excluded), the mixture blown with air to remove excess H2O, evaporated, the residue extracted with EtOH, the extract concentrated, and the precipitate (3 g.) repeatedly recrystd. from 70% EtOH with C gave 2.6 g. 4-NH2 derivative of III, m. 278-80° (decomposition) (70% EtOH). I (5.2 g.) and 7.5 g. I(CH2)3SO2NH2 in 9 cc. Ia kept 2 hrs. at 115-20° (oil bath), Ia decanted, the residual solid neutralized with aqueous NaHCO3, and recrystd. from 40% EtOH gave 1.3 g. 4-(3-sulfamoylpropyl) derivative of I, m. 177-9° (aqueous EtOH). I (8.7 g.) and 6.9 g. 4-hydroxy-1-butanesulfonic acid sultone (b14 151-2°) heated 1.5 hrs. at 165-75° (oil bath), cooled, and the product recrystd. from EtOH gave 9.5 g. 2-(4-sulfobutyl) derivative of I, m. 227-8° (90% EtOH).

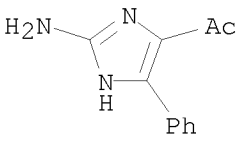
IT 96776-18-0
(Derived from data in the 7th Collective Formula Index (1962-1966))

RN 96776-18-0 CAPLUS

CN Ethanone, 1-(2-amino-4-phenyl-1H-imidazol-5-yl)-, nitrate (1:1) (CA INDEX NAME)

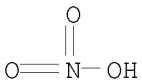
CM 1

CRN 96776-17-9
CMF C11 H11 N3 O



CM 2

CRN 7697-37-2
CMF H N O3



L10 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1939:8721 CAPLUS
DOCUMENT NUMBER: 33:8721
ORIGINAL REFERENCE NO.: 33:1319c-i,1320a-b
TITLE: Some new azo compounds and iodine derivatives of histidine and histamine
AUTHOR(S): Diemair, Willibald; Fox, Hermann
SOURCE: Berichte der Deutschen Chemischen Gesellschaft [Abteilung] B: Abhandlungen (1938), 71B, 2493-9
CODEN: BDCBAD; ISSN: 0365-9488
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

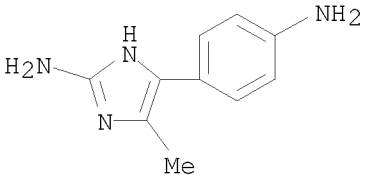
AB Under certain, exactly defined conditions, the Pauly reaction can be used for the determination of histidine and histamine. Attempts to isolate the dyes formed in the reaction had been unsuccessful (C. A. 32, 9136.1). The amino group in histidine was accordingly benzoylated by the Schotten-Baumann method (cf. Gerngross, C. A. 14, 2162) and the Nα-benzoylhistidine (I) converted into the Me ester (II). II couples with PhN2Cl to a crystalline homogeneous azo compound; during the coupling the ester grouping is cleaved and the product is bisphenylazo-Nα-benzoylhistidine, HO2CCH(NHBz)CH2C:C(N2Ph).NH.C(N2Ph):N (III); CH2N2 gives the Me ester (IV). The coupling of azo compds. with secondary cyclic amines proceeds through a diazoamino compound which rearranges secondarily into the true azo compound The rearrangement is rapid, so that several azo compds. can be formed at once; after the 1st rearrangement (and hence regeneration of the free imino group) a further mol. of PhN2Cl couples in the same way, etc. The side chain of the imidazole probably influences the rearrangement velocity so that in the presence of a carboxyl group in the side chain (histidine) only a bisazo compound is formed, and in that of an aliphatic side chain with no carboxyl group (histamine) only a monoazo compound is formed; Nα-benzoylhistamine gives a monophenylazo compound (V). p-Substitution in the diazo component seems to have a similar influence. p-O2NC6H4N2Cl with imidazole gives p-nitrophenylazoimidazole (VI); with IV in Na2CO3 it yields bis-p-nitrophenylazo-Nα-benzoylhistidine (VII). 2-Phenylazo-4-methylimidazole with SnCl2 in HCl undergoes a benzidine-like rearrangement to 2-amino-5-p-aminophenyl-4-methylimidazole (Fargher and Pyman, C. A. 13, 1301) and a similar reaction was to be expected in the reduction of III, but reductive cleavage of III and V showed that the expected amino compds. are very unstable. With SnCl2-HCl III gave a red HCl salt, very sensitive to air, of the aminohistidine. Al-Hg was not sufficiently powerful to completely decolorize III. On catalytic hydrogenation, by rapid work in the absence of air it was possible to obtain a crude amino-Nα-benzoylhistidine which, however, immediately decomposed into red oily smears on attempts to purify it or to stabilize the amino group (benzoylation according to Schotten-Baumann and in absolute pyridine, methylation with MeI, condensation with Me2NC6H4CHO, precipitation with picric acid). The difficulty is due to immediate decomposition of the imidazole nucleus, for when the SnCl2-HCl reduction product was allowed to stand only NH4Cl could be recovered. The instability of the amino derivs. of histidine is to be ascribed to the accumulation of amino groups on the imidazole nucleus. Reduction of V yielded a product separating from alc. in ill-defined crystals but rapidly decomposing on short standing in the air; benzoylation in CHCl3 gave no definite product. The formation of the monophenylazo compound of V led to attempts to substitute in histidine, in

addition to the 4(or 5) -position (alanine residue), a further (2- or 5(4))-C atom. By a modification of Pauly's method of iodination (C. A. 4, 2932) there was obtained an Nα-benzoyliodohistidine (VIII), which, as well as its Me ester (IX), is stable toward concentrated alkalies and moist Ag2O. The more striking and surprising, therefore, was its behavior on coupling with PhN2Cl in Na2CO3 solution The I was split off and III (or IV) was formed in good yield. Pauly's di-I compound behaves in the same way. III, cinnabar-red needles, is obtained in 2.4 g. yield from 1.35 g. II in 50 cc. of 10% Na2CO3 with 10 aqueous PhN2Cl. IV (75%), m. 217°. V, yellow, m. 186.5°. VI (20%), orange, m. 248°. VII, m. 162°; Me ester, fine powder, m. 208°. IX, from II in cold 0.1 N NaOH-MeOH with 0.1 N I, m. 190°; in aqueous 0.1 N I is obtained VIII, m. 208°.

IT 245547-21-1P, Imidazole, 2-amino-5-(p-aminophenyl)-4-methyl-
RL: PREP (Preparation)
(preparation of)

RN 245547-21-1 CAPLUS

CN 1H-Imidazol-2-amine, 5-(4-aminophenyl)-4-methyl- (CA INDEX NAME)



L10 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1919:6989 CAPLUS
DOCUMENT NUMBER: 13:6989
ORIGINAL REFERENCE NO.: 13:1301f-i,1302a-i,1303a-i,1304a-b
TITLE: Nitro-, arylazo-, and aminoglyoxalines
AUTHOR(S): Fargher, Robert George; Pyman, Frank Lee
CORPORATE SOURCE: Welcome Chem. Res. Lab., London
SOURCE: Journal of the Chemical Society, Transactions (1919), 115, 217-60
CODEN: JCHTA3; ISSN: 0368-1645
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C. A. 10, 1631. All m. ps. are corr. The object of this investigation was to prepare purine derivs. by building up a pyrimidine ring upon a glyoxaline nucleus, a method complementary to the usual one. It was proposed to prepare 4-aminoglyoxaline-5-carboxylic acid, CH:N.C(NH2):C(CO2H).NH, condense it with HCNO and obtain xanthine. The synthesis was not accomplished because of inability to obtain the starting material. I. The preparation of glyoxalines and their carboxylic acids: Glyoxaline-4,5-dicarboxylic acid (a), prepared in 60% yield by mixing cold aqueous solns. of nitrotartaric acid and CH2O, m. 288° (decomposition). Mono-sodium salt, forms feathery needles containing 1 H2O. Glyoxaline (b) is prepared by distilling (a) in small quantities at a time; picrate, yellow needles containing 1 H2O, m. 212°; hydrogen tartrate, anhydrous prisms, m. 202°; hydrogen oxalate, anhydrous prismatic needles, m. 232°. On heating (a) to above 180° with H2o or HCL the main product is (b) with a little glyoxaline-4-carboxylic acid. When (a) is heated to 180-200° with concentrated NH4OH the main product is (b). On boiling (a) with PhNH2 the main product is glyoxaline-4-carboxanilide, anhydrous needles, m. 227-8°, hydrolyzed by 10% HCl at 130°, producing glyoxaline-4-carboxylic acid.
2-Methylglyoxaline-4,5-dicarboxylic acid (c) is prepared from AcH and

nitrotartaric acid in 67% yield. On boiling (c) with PhNH2 there is obtained 11 g. 2-methyl-glyoxaline-4-carboxanilide (d), m. 208°, and 3.8 g. 2-methylglyoxaline; picrate, anhydrous needles from H2O, m. 213°; hydrogen oxalate, rhombic prisms from H2O containing 2 H2O; after drying at 100° it m. 160°. Hydrolysis of (d) gives 2-methylglyoxaline-4-carboxylic acid as a monohydrate, prismatic needles, m. 262° (decomposition); nitrate, rhombic prisms from H2O, m. 190°; picrate, minute cubes containing 2H2O, m. 200°. 2-Ethylglyoxaline-4,5-dicarboxylic acid, prepared from EtCHO and nitrotartaric acid in 64% yield, m. 259° (decomposition). 2-Phenylglyoxaline-4,5-dicarboxylic acid, from BzH and nitrotartaric acid in 48% yield, m. 271° (decomposition). When distilled in small quantities it gives an 80% yield of 2-phenylglyoxaline, needles from H2O, m. 148-9°; nitrate, leaflets from alc. containing 0.75 H2O, m. (dry) 135°; hydrogen oxalate, needles, m. 219° (decomposition); picrate, fine needles, m. 238°. Upon mixing 8.6 g. Ac2 in 50 cc. H2O, 50 cc. of 40% aqueous CH2O, and 80 cc. concentrated NH4OH at 0° there is obtained after standing in a cool place overnight, evaporating to a small bulk, saturating with K2CO3, extracting with Et2O, and evaporating the extract, 5.9 g. of an oil which is boiled with dilute HCl to destroy C6H12N4 and separated by fractionating the picrates from H2O into 5.7 g. 4,5-dimethylglyoxaline picrate (e), and 3.5 g. 2,4,5-trimethylglyoxaline picrate, m. 163°. 4,5-Dimethylglyoxaline hydrochloride forms rhombic prisms from H2O, m. 305° (decomposition). (e) is also prepared from MeCOC(:NOH)Me (9 g.) by reducing with SnCl2 at is 15° and evaporating the final liquor under reduced pressure; the resulting 10 g. MeCOCH(NH2)Me heated on the H2O bath 4 hrs. with 10 g. KCNS and 40 cc. H2O gives 5.2 g. 2-thiol-4,5-dimethylglyoxaline and the latter gives an 85% yield of (e) when oxidized with the calculated quantity of FeCl3. II. Nitroglyoxalines: 4-Nitroglyoxaline (f) is obtained in 63% yield when 8 g. of (b) in 16 cc. cold HNO3 (1.4), is cautiously treated with 16 cc. H2SO4, and after the vigorous reaction is over boiled 2 hrs. and poured into ice-H2O. 4-Nitro-2-methylglyoxaline, (g), prepared similarly, anhydrous needles from H2O, sinter 251°, m. 254°. On nitrating 4-methylglyoxaline by the method of Windaus (C. A. 3, 1268) the main product is 4-methylglyoxaline nitrate instead of 5-nitro-4-methylglyoxaline (h) as stated by him. (h), obtained in 90% yield by the method described for preparing (g), m. 248°. On attempting to nitrate 4,5-dimethylglyoxaline (5 g.) with HNO3 and H2SO4 1.7 g. was recovered unchanged and the only product was 0.3 g. of the nitrate of 4-methylglyoxaline-5-carboxylic acid. When (f), (g), or (h) are reduced with Sn and HCl two of the three atoms of N present are eliminated as NH3. Three mols. (f) on reduction with alkaline Na2S2O4 loses 2 atoms N as NH3. The remaining liquor gradually acquired a blue color as noted by Behrend and Schmitz (Ann. 277, 338) and on acidification precipitated less than 0.1 g. of a blue compound m. above 300°. (h) on reduction behaved analogously but gave a rose color and no precipitate (g) gave 1 mol. of NH3 from 3 mols. of the nitro-compound III. Arylazoglyoxalines: In the opinion of the authors it appears that glyoxalines, in order to be capable of coupling, must contain a free « NH group and also a H atom or some other displaceable group, such as CO2H, in one of the 2-, 4-, or 5-positions. All previously prepared arylazoglyoxalines are C-azo compds. In general, the monoarylazoglyoxalines are soluble in alc., EtOAc and Me2CO, sparingly soluble in Et2O, CHCl3 and C6H6, insol, in cold H2O and dilute alkali, form soluble salts with dilute HCl; are decomposed by boiling 1 hr. with 10% HCl, give bright colors with concentrated H2SO4. 17 g. (b) and 40 g. Na2CO3 in 125 cc. H2O treated at 5° with a diazotized solution of 23.25 g. PhNH2 give an orange powder which, on extracting with cold 2.5% HCl, left 4.4 g. residue of 2,4,5-trisbenzeneazoglyoxaline, decomps. about 200°,

effervesces 208°. The HCl extract made alkaline gave 34 g. 2-benzeneazoglyoxaflne (i), m. 190°. 20 g. of (i) reduced with $SnCl_2$ gives 3.2 g. 2-aminoglyoxaline, chlorostannate, a trace of $NH_2C(:NH)NH_2$, and 18.55 g. 2-amino-4-p-aminophenylglyoxaline dihydrochloride (j), formed by rearrangement of the benzidine type, m. above 300°; free base, formed by boiling with Na_2CO_3, glistening leaflets containing 1 H_2O, m. 148°; dipicrate, yellow needles, darken 245°, M. 250° (decomposition). 2-Acetylamino-4-p-acetylaminophenylglyoxaline, by boiling the base with Ac_2O 1 hr., crystalline powder, m. above 300°. 10 g. in dilute H_2SO_4 with 4% $KMnO_4$ gave 1 g. p-$AcNHC_6H_4CO_2H$, m. 260°. Reduction of 17.2 g. (i) with Zn dust and AcOH gives a small amount of (j), 7 g. $PhNH_2$, and 5.9 g. of pure glycocyamidine hydrochloride (k), sintered 205°, m. 211-3°; free base, prismatic needles. begins darkening 220° and does not m. 300°; chloroplatinate, $C_3H_5ON_3.H_2PtCl_6.2H_2O$, darkens 220°, entirely black at 260°, does not m. 300°; chloraurate, $C_3H_5ON_3.AuCl_3$, m. 157-8°; picrate, yellow leaflets, m. 215-16°. By treating 13.6 g. (b) in Na_2CO_3 at 5° with a diazotized solution of 34.4 g. p-$BrC_6H_4NH_2$ there resulted 48.7 g. crude 2-p-bromobenzeneazoglyoxaline (l); crystallization from alc. gave 42.6 g. of the pure compound m. 253° (decomposition) and a small amount of 4-p-bromobenzeneazoglyoxaline, m. 191° (decomposition). (l) (78 g.) on reduction with $SnCl_2$ gave 40.7 g. p-$BrC_6H_4NH_2$, 2.7 g. of 2-amino-4-p-aminophenylglyoxaline, isolated as the picrate, 1.6 g. $NH_2C(:NH)NH_2.(CO_2H)_2$, m. 173-4°, 0.9 g. of a base forming needles, m. 178°, probably having the structure 5,2-$Br(H_2N)C_6H_3NHC:N.CH:CH.NH$, and 20.7 g. 2-aminoglyoxaline hydrochloride (m), plates from alc., m. 152°; free base, obtained as a colorless sirup by adding 1 equivalent of Na_2CO_3, evaporating to dryness, extracting with alc., and evaporating the alc.; chlorostannate, prismatic needles, m. 286°; nitrate, transparent tablets, sinter 125°, m. 135-6°; hydrogen oxalate, tablets, m. 211°; picrate, silky needles, m. 236°. 2-Acetylaminoglyoxaline, prepared by boiling (m) with Ac_2O and AcONa, prisms, sinter 270°, m. 287°. 2-Benzoylaminoglyoxaline, prepared by Schotten-Baumann reaction, leaflets, m. 227°. 4-Methylglyoxaline (32.8 g.) in $NaHCO_3$ treated with PhN:NCl gave 17.3 g. 2,5-bisbenzeneazo-4-methylgtyoxaldne, garnet-red needles from alc., m. 206° (decomposition); 17 g. of 5-benseneazo-4-methylglyoxaline (n), copper-colored needles, m. 240° (decomposition); 7.4 g. of 2-benzeneazo-4-methylglyoxatine (o), orange prisms, m. 185°. Reduced with $SnCl_2$ (o) gives 2-amino-5-p-amixophenyl-4-methylglyoxaline dihydrochloride (p), diamond-shaped plates, m. above 300°. (p) boiled with Na_2CO_3 gives the monohydrochloride, flat needles, sinter 80°, m. 260°; dipicrate, yellow needles, m. 255°. 2-Acetylamino-5-p-acetylaminophenyl-4-methylglyoxaline hydrochloride, prepared by the action of Ac_2O and AcONa on (p), needles containing 4 H_2O, after drying at 100° m. 303° (decomposition). On adding NH_4OH to the solution of the hydrochloride the free base is precipitated, needles, m. 280°. 2-Amino-5-p-benzylideneaminophenyl-4-methylglyoxali neacetate, prepared by adding BzH to (p) in AcONa solution, m. 208°. (o) on reduction with Zn and AcOH gave 1.4 g. brown sirup from which was separated a small quantity of the dipicrate of (p) and about 0.7 g. alacreatinine hydrochloride, prisms, m. 202-3°; free base, m. 222-3°; picrale, yellow needles, sinter 200°, m. 212°. On reduction of 14 g. of (n) with $SnCl_2$ there is obtained besides $PhNH_2$ and a brown gum, 2.2 g. of the hydrochloride, $C_9H_{10}ON_2.HCl$, rectangular tablets, m. 308°, from which a base, $C_3H_{10}ON_2$, is obtained by adding NH_4OH and crystallizing from H_2O, prisms, m. 185°. Reduction of 10. g. (n) with Zn and AcOH produced 5.5 g. of a varnish-like substance and 1.6 g. of the

base C10HON3, small, rhomboidal plates, m. 265°; hydrochloride, oblong plates, m. 206-8°, decomposed by heating 2.5 hrs. at 170° into NH4Cl and a hydrochloride, m. about 280°. 2-Methylglyoxaline in Na2CO3 treated with PhN:NCl gives a product which easily resinifies and from which a small amount of 4-benzeneazo-2-methylglyoxaline was obtained pure, m. 158°. 4-p-Bromobenzeneazo-2-methylglyoxaline, prepared in good yield from 2-methylglyoxaline in Na2CO3 and p-BrC6H4N:NCl, red prism sfrom absolute alc., m. 200° (decomposition); reduction with either SnCl2 or Zn and AcOH give no definite products. 2-Phenylglyoxaline (7.2 g.) heated with p-BrC6H4N:NCl gives 13 g. 2-phenyl-4-p-bromobenzeneazoglyoxaline (q), orange needles, m. 201°. Reduction of (g) with SnCl2 gives a crystalline hydrochloride, C15H13N4Br.2HCl, m. 255°; triacetyl derivative, formed by heating with Ac2O and AcONa, m. above 300°. This base is probably the result of a change of the semidine or benzidine type. 2-p-Sulfobenzeneazoglyoxaline-4,5-dicarboxylic acid, prepared by treating glyoxaline-4,5-dicarboxylic acid with SO3HC6H4N:NCl, red prisms containing 2 H2O which are lost at 130° in vacao; disodium salt (r), yellow, silky needles containing 3 H2O. Reduction of 6.2 g. (r) with Na2S2O4 gives 1.6 g. of 2-aminoglyoxaline-4,5-dicarboxylic acid, pale buff needles, effervesce 245° and then melt. On boiling 6 hrs. with PhNH2 the product was identified as (m).

IT 245547-21-1, Imidazole, 2-amino-5-(p-aminophenyl)-4-methyl- (derivs.)

RN 245547-21-1 CAPLUS

CN 1H-Imidazol-2-amine, 5-(4-aminophenyl)-4-methyl- (CA INDEX NAME)